Supporting Information

Isomeric Organic Semiconductors Containing Fused-Thiophene Cores: Molecular Packing and Charge Transport

Dongfeng Dang, a,c * Pei Zhou, c Yong Wu, a Yanzi Xu, a Ying Zhi, a Weiguo Zhu b,c *

a School of Science, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiao Tong University, Xi'an 710049, P. R. China.

b School of Materials Science and Engineering, Changzhou University, Changzhou 213164, P. R. China.

c Department of Chemistry, Key Lab of Environment-Friendly Chemistry and Application in the Ministry of Education, Xiangtan University, Xiangtan 411105, P. R. China.

Corresponding author:

Dr. Dongfeng Dang and Prof. Weiguo Zhu

E-mail addresses: zhuwg18@126.com; dongfengdang@mail.xjtu.edu.cn

Fig. S1. The UV-Vis spectra of TF1 and TF2 in gas phase by TD-DFT.
Fig. S2. The UV-Vis spectra of TF1 (a) and TF2 (b) in o-DCB solution at 25° and 50°.

Fig. S3. The UV-Vis spectra of TF1 (a) and TF2 (b) in thin films with and without annealing (140° and 120° for TF1 and TF2, respectively).

Fig. S4. The X-ray diffractions of TF1 and TF2 in thin films.
Fig. S5. Output (a, c) and transfer (b, d) characteristics of TF1 and TF2-based OFETs devices at room temperature.

Table S1. Optical properties of TF1 and TF2.
### Scheme S1. Synthetic routes of TF1 and TF2.

![Scheme S1](image)

### Synthesis of TF1 and TF2

In a 50 mL two-neck flask, tetrakis-(triphenylphosphine)palladium(0) \([\text{Pd(PPh}_3\text{)}_4]\) (10 mg) was added to the solution of tributyl-(5-octyl-thiophen-2-yl)-stannane (63.6 mg, 0.13 mmol) and M1 (50.1 mg, 0.05 mmol) in 30 mL toluene under nitrogen and then stirred at 110 °C overnight. After cooled downed to room temperature (RT), the solvent was removed under reduced pressure and then poured into methanol to get the precipitation. Finally, TF1 was purified through recrystallization by using THF and ethanol as dark-orange solid (44.6 mg, 68.6%). \(^1\text{H NMR (400 MHz, CDCl}_3\text{)}\) \(\delta\) (ppm), 7.49 (s, 2H), 7.04 (s, 2H), 6.99 (s, 2H), 2.90–2.80 (m, 8H), 2.80–2.70 (m, 4H), 1.85–1.70 (m, 8H), 1.58–1.29 (m, 64H), 0.95–0.80 (m, 18H). MS (MALDI-TOF) m/z: M\(^+\) calculated for C\(_{78}\)H\(_{108}\)S\(_8\), 1300.6, found 1300.9.

The synthetic procedure to TF2 is similar to that of TF1 with a yield of 78.5% as bright yellow solid. \(^1\text{H NMR (400 MHz, CDCl}_3\text{)}\) \(\delta\) (ppm), 7.27 (s, 2H), 7.06 (s, 2H), 6.70 (s, 2H), 3.41–3.30 (m, 4H), 2.89–2.78 (m, 8H), 1.76–1.60 (m, 12H), 1.58–1.25

### Table

<table>
<thead>
<tr>
<th>Compounds</th>
<th>UV (\lambda_{\text{abs}}) [a] (nm)</th>
<th>UV (\lambda_{\text{abs}}) [b] (nm)</th>
<th>PL (\lambda_{\text{em}}) [a] (nm)</th>
<th>PL (\lambda_{\text{em}}) [b] (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TF1</td>
<td>300, 428, 457</td>
<td>300, 424, 454, 483</td>
<td>465, 493, 530</td>
<td>565</td>
</tr>
<tr>
<td>TF2</td>
<td>308, 433, 455</td>
<td>312, 428, 448, 480</td>
<td>472, 499, 533</td>
<td>567</td>
</tr>
</tbody>
</table>

[a] In solution; [b] In films.
(m, 60H), 0.98–0.81 (m, 18H). MS (MALDI-TOF) m/z: M+ calculated for C_{78}H_{108}S_{8}, 1300.6, found 1301.0.

NMR and MALDI-TOF spectra
1300.9